Classical Mechanics and Quantum Mechanics

Review of Fundamentals of Classical Mechanics (Canonical Formalism):

- Canonical Variables \( q_i, p_i \)
  A complete description of physical system

- Hamiltonian \( H(q, p, t) \) determines dynamics (time-evolution)

- Least Action Principle \( \delta \left[ \int L(q, q', t) dt \right] = 0 \)
  i.e. \( \delta S_H = 0 \)

- Canonical Eqs: \( \dot{q}_i = \frac{\partial H}{\partial p_i} \); \( \dot{p}_i = -\frac{\partial H}{\partial q_i} \)
  (Central Problem: Integrate these eqns)

- Dynamical Variables \( A(q, p, t) \)

- Poisson Bracket \( \{A, B\} = \text{Lie Algebra structure for dynamical variables. They can be derived from canonical brackets} \)
  \( \{q_i, q_j\} = \{p_i, p_j\} = \{q_i, p_j\} = 0 \)

- Time evolution of dynamical variable:
  \( \frac{\text{d}A}{\text{d}t} = \{A, H\} + \frac{\partial A}{\partial t} \)

- Canonical Transformation \( H, q, p \rightarrow K, Q, P \)
  \( Q_i = \frac{2K_i}{p_i} \); \( P_i = -\frac{2K_i}{q_i} \)
  \( \{Q_i, P_j\} = \delta_{ij} \delta_{Q}\text{c}\) 

- \( G \) (q, p, t):
  \( P = 26/2q; \); \( Q = 26/2p; \); \( K = N + 1/2 \text{c} \)

- Infinitesimal Canonical Transformation
  - Generated by \( G^x(q, p, t) \); \( \delta A = \varepsilon \{A, G^x\} \)
  (Time evolution is a canonical trans generated by \( H \))

- Symmetries
  Inf. canon. trans. generated by \( G^y(q, p) \) leaves \( H \) invariant
  \( \{H, G^y\} = 0 \Rightarrow G^y \text{ is conserved} \)

- H-J Theory:
  \( \frac{\partial}{\partial t} \frac{\partial S}{\partial (q, t)} + H(q, \frac{\partial S}{\partial (q, t)}, t) = 0 \), then
  \( S \) generated canonical trans. such that \( Q, P \) are constant
  \( S \) = action as function of \( Q, P \) coordinates

- Separable problems + action-angle variables
  Multiply possible N terms in \( 2N \) dim phase space

- No of one-valued constants of motion \( \Rightarrow \) \( 2N \) minus dimensionality of system manifold
Fundamentals of Quantum Mechanics (Quantization): To quantize a classical system, how do we quantize it?

- **Hilbert Space**: complex inner product space, the arena of QM
  \[(\phi, \psi) = (\psi, \phi)^* = \phi^* \psi, \phi, \psi \in \mathcal{H}\]

- States of a QM system = rays in Hilbert space \(\mathcal{H}\) with unit length, arbitrary phase

- **Observable (dynamical variable)** is a hermitian linear (actually self-adjoint) operator in Hilbert space $E.g.$ $\hat{A}$, $\hat{P}$

  What is the connection of these operators to outcomes of a measurement?

  Observable $\hat{A}$ has basis of eigenvalues $\hat{A} \psi_a = \lambda_a \psi_a$

  $\psi = \sum a \lambda_a \psi_a$, $\frac{1}{\hat{A}} = \sum a \lambda_a^2 = 1$

  Then if $\hat{A}$ is measured for state $\psi$, $\left| \lambda_a \right|^2$ is probability

  Most outcome is $\lambda_a$.

  In state $\psi$, expectation value of $\hat{A}$ is

  $\langle A \rangle = \sum_a \lambda_a \left| \lambda_a \right|^2 = \langle \psi, \hat{A} \psi \rangle$

- **Dynamics** is determined by $H(q, p)$

  To explain how we must first consider ordering of operators

- **Commutators** (canonical quantization) operators (e.g. matrices) do not commute. How do we assign commutators when we want to quantize a system?
\[ [A, B]_{\text{comm}} = \frac{1}{i\hbar} [A - B] \]

Note that \( [A, B]_{\text{comm}} \) has some algebraic properties as \( [A, B]_{\text{Enh}} \):

1. \( [aA, bB]_{\text{comm}} = (ab) [A, B]_{\text{comm}} \)
2. \( [aA + bB, C]_{\text{comm}} = a[A, C]_{\text{comm}} + b[B, C]_{\text{comm}} \)
3. \( [AB, C]_{\text{comm}} = A [B, C]_{\text{comm}} + [A, C]_{\text{comm}} \)
4. \( [A, B]_{\text{comm}} + [C, A]_{\text{comm}} + [C, B]_{\text{comm}} = 0 \)

(Lie Algebra of Observables)

It is consistent to assign commutators in the following way: Suppose \( A(\theta, \phi) \) is the same function of \( \theta, \phi \) that \( A(\theta, \phi) \) is of \( \theta, \phi \), and similar for \( B, C, \ldots \)

\[
\text{Then, if } [A, B]_{\text{comm}} = C, \text{ assign } [A, B]_{\text{Enh}} = i\hbar C
\]

\( \hbar = \text{Planck's constant} \)

This is consistent because both brackets obey rules (1)-(3) above. Hence any bracket can be reduced to the canonical brackets, e.g. \( \frac{\text{Take } \text{Kronecker} \times \text{Hilbert space to be 2-dimensional, etc.}}{E_i, \xi_i = -i\hbar \delta_i, \text{ etc.}} \)

One must be cautious about abusing ambiguities, however - e.g. \( \phi \phi \to \frac{1}{2} (\phi \phi + \phi \phi) : \text{hermitian} \)

It really suffices to specify \( \{\xi_i, \xi_i\} = 0 \) \( \{E_i, \xi_i\} = 0 \) \( \{E_i, E_j\} = i\hbar \delta_{ij} \)

These canonical commutation relations completely define the quantum mechanical system.

As \( \hbar \to 0 \), all observables commute.
- **Time Evolution**

  When we carry out canonical quantization, the Hamiltonian of the QM system becomes

  \[ H(t) = \mathcal{H} \]

  The classical eqn

  \[ \frac{dA}{dt} = [A, \mathcal{H}]_{PB} \] (time-independent dynamical variable)

  suggests

  \[ i\hbar \frac{dA}{dt} = \mathcal{H} \text{com} \]

  (Herschberg picture dynamics)

  The "correspondence principle" is built into this relation, because, if we take expectation values

  \[ i\hbar \frac{d}{dt} \langle A \rangle = \langle [A, \mathcal{H}] \rangle = i\hbar \langle \mathcal{E} \rangle \]

  where \( \mathcal{E} = [A, \mathcal{H}]_{PB} \).

  Thus, the expectation values of observables evolve like classical dynamical variables.

- **Unitary Transformations**

  \[ U = \mathcal{Q} \mathcal{P} U^+ \]

  \[ U U^+ = I \quad \text{Hermitian} \]

  \[ [\mathcal{Q}, \mathcal{P}]_{\text{com}} = \mathcal{U} [\mathcal{Q}, \mathcal{P}] U^+ = i\hbar \]

  Transformation is "canonical" - it preserves all poison brackets (canonical commutator).

  [One can also prove converse: If \( \mathcal{Q}, \mathcal{P} \) obey canonical relations, there is a unitary transformation \( \mathcal{U} \) taking \( \mathcal{Q}, \mathcal{P} \) to \( \mathcal{Q}, \mathcal{P} \). See Dirac, Principles of QM].

  All isopsonic relations unitarily equivalent - von Neumann

- **Infinitesimal Unitary Transformation**

  \[ U = \mathcal{I} + i \epsilon \mathcal{G} \]

  \[ U U^+ = \mathcal{I} = \mathcal{I} + i \epsilon (\mathcal{G} - \mathcal{G}^+) \]

  \[ U^+ = \mathcal{I} - i \epsilon \mathcal{G}^+ \]

  Infinitesimal unitary transformations are generated by observables (self-adjoint operators).
\[ A \rightarrow U A U^+ = A + i \hbar [G, A] \]

Note: time evolution is a unitary transformation generated by the Hamiltonian.

If \([G, H] = 0\), then unitary trans. generated by \(G\) leaves \(H\) invariant (symmetry) and \(\frac{d}{dt} G = 0\).

**Schrodinger Eq**

If \(H\) is not explicitly time-dependent, the canonical transformation which "stops" the motion of an observable is

\[ U(t) = e^{-iHt/\hbar}, \quad U(t) = e^{iHt/\hbar} \]

\[ \frac{d}{dt} U(t) = i\hbar H U \Rightarrow i\hbar \frac{d}{dt} U(t) = \frac{i}{\hbar} H U \]

\[ \frac{d}{dt} A = \frac{i}{\hbar} [A, H] = i\hbar \left( i\hbar \frac{d}{dt} C_{A, H} \right) + \hbar A - A H \int U^+ = 0 \]

But holding observables fixed causes states to move

\[ \vec{\psi} = U(t) \psi_0 \Rightarrow \frac{d}{dt} \vec{\psi} = \frac{i}{\hbar} H \vec{\psi} \quad \text{Schrodinger Eq} \]

**Schrodinger Representation**

Represent Hilbert Space by functions of the \(q_i\)

\[ \psi(q_1, \ldots, q_n, t) \]

\(q_i\) is multiplication by \(q_i\)

\(p_i = -i\hbar \frac{\partial}{\partial q_i}\) - gradient

\[ [q_i, p_j] = -i\hbar \delta_{ij} \]

\(\psi(x)\), for a particle in a potential \(H = \frac{\vec{p}^2}{2m} + V(x)\)

\[ H = \frac{\vec{p}^2}{2m} + V(x) \]
- Schrödinger Equation and Hamilton-Jacobi Theory

\[ i\hbar \frac{\partial \psi}{\partial t} = H(\mathbf{q}, \mathbf{p}) \psi \quad \psi = \psi(q, t) \]

Represent \( \psi = e^{iS/\hbar} \)

\[ i\hbar \left( \frac{\hbar}{\partial t} \right) e^{iS/\hbar} = H e^{iS/\hbar} \]

\[ \Rightarrow \quad - \frac{\partial S}{\partial t} = e^{-iS/\hbar} H e^{iS/\hbar} \]

\( S \) is a function of \( q \), and \( \mathbf{p} = -i\hbar \frac{\partial}{\partial q} \)

\[ \Rightarrow \quad - \frac{\partial S}{\partial t} = H(q, -i\hbar \frac{\partial}{\partial q} + \frac{\partial S}{\partial q}) \]

Now, if we take formal \( \hbar \to 0 \) limit

\[ \left[ \frac{\partial S}{\partial t} + H(q, \frac{\partial S}{\partial q}) \right] = 0 \]

The Hamilton-Jacobi equation is the classical limit of the Schrödinger equation.

What approximation are we really making? Consider, for concreteness, the case of a particle in one dimension

\[ H = \frac{p^2}{2m} + V(q) \]

\[ 0 = \frac{\partial S}{\partial t} + \frac{1}{2m} \left( -i\hbar \frac{\partial S}{\partial q} + \frac{\partial S}{\partial q} \right)^2 + V(q) \]

\[ \Rightarrow \left[ \frac{\partial S}{\partial t} + \frac{1}{2m} \left( \frac{\partial S}{\partial q} \right)^2 + V(q) \right] = i\hbar \frac{\partial S}{\partial q} \]

\[ \Rightarrow \quad \text{We have assumed} \quad \left( \frac{\partial S}{\partial q} \right)^2 \gg i\hbar \frac{\partial S}{\partial q} \]

\[ \Rightarrow \quad \frac{\partial}{\partial q} \left[ \frac{k(\frac{\partial S}{\partial q})^{-1}}{2m} \right] \ll 1 \]

But Hamilton-Jacobi \( \Rightarrow \frac{\partial S}{\partial q} = p \), so

\[ \frac{\partial}{\partial q} \left( \frac{k}{p} \right) \ll 1 \]

The deBroglie wavelength must change negligibly when \( q \) advances by one wavelength.
Thus, classical mechanics (H-J theory) is the short wavelength (or "geometrical optics") limit of quantum mechanics. Another way of saying it is, $\frac{\hbar}{\lambda}$, the phase of $\psi$ advances by a large amount when a small displacement is made.

E.g. bacterium

\[
\text{min } 10^{-8} \text{ grams } \quad S = \frac{4}{3} \pi r^3 \cdot \frac{1}{2} \cdot 10^{-8} \cdot 10^{-6} \cdot 5 \times 10^{-15} \text{ g/cm}^3 \\
5 \times 10^{-3} \text{ cm } \quad t = 1 \text{ sec} \\
\Rightarrow \frac{\hbar}{\lambda} = 5 \times 10^{12}
\]

Bacteria are classical.

Electron

\[
\text{min } 10^{-27} \text{ g } \quad S = \frac{4}{3} \pi r^3 \cdot \frac{1}{2} \cdot 10^{-27} \cdot 10^{-8} = \frac{1}{10} \text{ cm}^3 \text{ g}^{-1} \\
5 \times 10^{-3} \text{ cm } \quad V = 10^{-18} \text{ cm/sec} \\
\Rightarrow \frac{\hbar}{\lambda} = \frac{1}{10}
\]

Electrons are quantum mechanical.

Since $\psi = e^{iS/\hbar}$, where $S$ is the classical action

\[ p \psi = \frac{\partial}{\partial q} \psi = p \psi \]

In the Schrödinger 

\[ \text{vop, } p \] like $i$ is just a multiplication operator observables become numbers in the classical limit.

The H-J theory is just the first term in a systematic expansion in powers of $\hbar$ for $S$ (called the "semiclassical" or "WKB" expansion).

\[ S = S_0 + \frac{\hbar}{2} S_1 + \cdots \quad \text{or} \quad S = -Et + W_0 + \frac{\hbar}{2} W_2 \]

Consider e.g. a particle in one dimension. We know from solving the H-J eqn for

\[ H = \frac{p^2}{2m} + V(q) \quad \text{Eqs. (7.9)} \]

Then

\[ S_0 = \pm \int p dq - Et \quad \text{and} \quad p = \sqrt{2m(E-V)} \]

$W_0$ = Hamilton's characteristic function = Mayer's action.

If we retain corrections of order $\hbar$ in the Schrödinger eqn,
\[
\frac{d\psi}{dt} + \frac{1}{2m} \left( \frac{d\psi}{dq} \right)^2 + V(q) = \frac{i\hbar}{2m} \frac{d^2\psi}{dq^2}
\]

\[ \Rightarrow \frac{1}{2m} \left( \frac{dW_0}{dq} + \frac{2\hbar}{i} \frac{dW_1}{dq} \right) + V - E = \frac{i\hbar}{2m} \frac{d^2W_0}{dq^2} \]

\[ \Rightarrow -\frac{dW_1}{dq} = \frac{i\hbar}{p} \frac{dF}{dq} \]

\[ dW_1 = \frac{-i\hbar}{p} dq \Rightarrow W_1 = -\frac{i\hbar}{p} \ln p + \text{const} \]

\[ \exp(W_1) = C p^{-\frac{1}{2}} \]

\[ \Rightarrow Y = C p^{-\frac{1}{2}} \exp\left( \frac{i\hbar}{\hbar} \int p dq \right) [1 + O(\hbar)] \]

\[ \times e^{-iEqt} \]

The \( p^{-\frac{1}{2}} \) is easy to interpret, since we have

\[ |Y| \propto \frac{1}{p} x \frac{1}{V} \]

- This is the expected behavior for a classical trajectory.

The probability \( 141 \frac{dq}{dq} \) of finding particle between \( q \) and \( q+dq \) is proportional to the time the classical particle spends there.

[To establish a connection between classical motion
and the Schrödinger eqn, we need to construct narrow wave packets, and note that they evolve like classical particles, with negligible spreading of the packet for \( \hbar \) sufficiently small.]

\[ \text{Note: Probability appears to diverge near endpoints:} \]

\[ |Y| \] This is actually wrong; the quasiclassical approach always breaks down near the endpoints, because wavelength changes rapidly. The resolution of this problem is discussed in advanced QM texts, e.g. L&L.

\[ A \text{ further bonus: WKB works in classically forbidden regime} \]
Propagation of a wave packet

Consider the particle in one dimension

\[ \psi(q,t) \sim e^{i(\frac{p_q}{\hbar} - Et)/\hbar} \]

If we consider a "surface of constant phase," we have

\[ pdq - E dt = 0 \quad \Rightarrow \quad \frac{dq}{dt} = \frac{E}{p} \]

The surface of constant phase advances at a rate

\[ \nu_{\text{phase}} = \frac{E}{p} \quad \Rightarrow \quad \nu_{\text{phase}} \propto \text{velocity} \]

To see the correspondence with classical motion more clearly, we should consider the evolution of a narrow wave packet

\[ \psi(q,t) = \int dp \phi(p) e^{i(p_q - E_0 t)/\hbar} \]

where \( \phi(p) \) is sharply peaked about \( p = p_0 \), with width \( \sim dp \)

Expand \( E_0 + (p - p_0) \frac{dE}{dp} + \frac{1}{2} (p - p_0)^2 \frac{d^2E}{dp^2} \)

\[ \approx e^{i(p_0 q - E_0 t)/\hbar} \int dp \phi(p) \exp \left[ i(p - p_0) \frac{q - dE}{dp} t/\hbar \right] \]

\[ - i \frac{t}{\hbar} (p - p_0) \frac{d^2E}{dp^2} \]
We can ignore higher order corrections in the exponent as long as

\[
\frac{1}{2} (\Delta p)^2 \frac{d^2 E}{dp^2} t \ll 1
\]

Then except for an overall phase

\[
\int \Rightarrow \quad \text{the wave in } q \text{ space is translated without changing shape}
\]

It moves according to

\[
\Delta q = \frac{dE}{dp} \Delta t \quad \text{or} \quad \frac{\partial}{\partial q} = \frac{\partial H}{\partial p}
\]

— Hamilton's equation

To understand the approximation

\[
V = \frac{dE}{dp} \Rightarrow \text{Kerr's velocity dispersion}
\]

\[
\Delta V = \frac{d^2 E}{dp^2} \Delta p
\]

This leads to significant "spreading" of the wave packet after time \( t \) if

\[
t \Delta V \sim \Delta x \quad \text{or, from the uncertainty relation} \quad \Delta x \sim \frac{\Delta p}{\mu}
\]

Kerr is

\[
\frac{t}{\mu} \Delta u \Delta p \ll 1
\]

or \( (\Delta p)^2 \frac{d^2 E}{dp^2} \frac{t}{\mu} \ll 1 \) — So the condition found above is a condition for spreading to be negligible
we can generalize this discussion to a general system with time-independent Hamiltonian: Hamilton-Jacobi eqn is solved by

$$ S = W(q) - ET $$

where \( \frac{\partial W}{\partial q_i} = p_i \)

So the Schrödinger eqn in geometrical optics is

$$ \psi(q, t) \sim \exp[i(W(q) - ET)] $$

First consider surfaces of constant phase (in configuration space)

$$ W(q) = ET + \text{constant} $$

Since

$$ \nabla W = \mathbf{p} \quad \text{and} \quad \nabla W \text{ is orthogonal to surfaces of constant } W \quad \text{we see that momentum points} \quad \text{to surfaces of constant } W $$

The rate at which this surface moves is

$$ |\nabla W| (dq) = EAT $$

$$ V_{phase} = \frac{E}{|\nabla W|} = \frac{E}{P} $$

But if we consider a wave packet, say of the form

$$ \psi \sim \text{Sdp } \phi(p) \exp[i(W(q) - ET)/\hbar] $$
we again consider expanding around $P_0$ where $\phi(p)$ is peaked

$$E_t = E_0 + (\vec{P} - \vec{P}_0) \cdot \vec{\nabla}_P E_t$$

But we note that

$$W(\vec{q} + \delta \vec{q}) = W(\vec{q}) + \delta \vec{q} \cdot \vec{\nabla}_q W$$

Thus we can absorb the linear term in $(\vec{P} - \vec{P}_0)$ into a shift in $\vec{q}$ by

$$\delta \vec{q} = \vec{\nabla}_P E_t$$

Thus, the center of the wave packet propagates according to

$$\dot{\vec{q}} = \frac{1}{\hbar} \vec{p}; \qquad H \quad \text{Hamilton's equation}$$

To see that the other Hamilton eqn is also satisfied, we may again consider evolution of a wave packet in momentum space.